Turbulent Mixing Simulations with Verification and Validation

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Turbulent mixing is central to a number of LANL problems, including inertial confinement fusion (ICF) and turbulent combustion. Classic acceleration-driven instabilities (Rayleigh-Taylor for continuous acceleration and Richtmyer-Meshkov for shock acceleration) have been a numerical challenge for 50 years. A satisfactory solution should use a compressible code, satisfy verification and validation (V&V) standards, achieve mesh-converged probability distributions for temperature and mixture concentrations, not require full resolution direct numerical simulation (DNS) of all turbulent length scales, apply over a range of physical parameters, including high Schmidt numbers, and provide sufficient intellectual understanding that others can follow and improve.

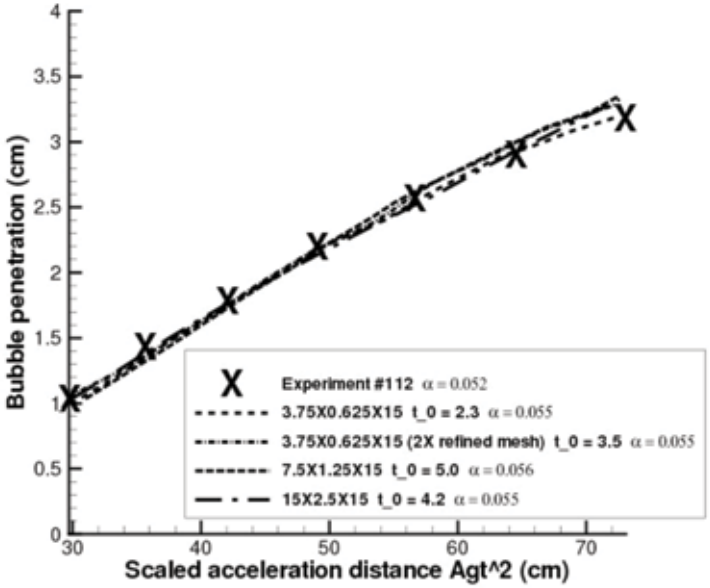

Fig. 1. Smeeton-Youngs experiment #112 (salt-fresh water) compared with several simulations with different mesh and statistical resolutions.

Our progress report, based on recent results from a LANL-Stony Brook University collaboration, outlines results that achieve these six goals.

The compressible code is the LANL-Stony Brook code FronTier, whose main two innovative features are front tracking, to eliminate numerical mass diffusion across fluid interfaces, and dynamic subgrid scale (SGS) models, to represent turbulent fluctuations at levels below the grid resolution.

The SGS models are free of adjustable parameters, and the entire simulation is thus free of adjustable parameters. Such SGS models are standard, but our use of them in flows with flow gradients that are strong at a mesh level appears to be original.

The main results are contained in a series of recent papers [1-4]. The summary here will emphasize the sixth point—the intellectual and conceptual innovations needed (going beyond the capabilities of an advanced computer code) to obtain these results.

Commonly, the Rayleigh-Taylor mixing simulations show a factor of two or more discrepancy between simulation and experiment. Conventionally, this discrepancy is attributed to long wavelength noise in the experiments, but not measured – hence the simulations and (most) experiments should not be compared. The Mueschke-Andrews experiments (hot-cold water flowing over a splitter plate) are an exception—measured initial data shows very substantial long wavelength initial perturbations. We duplicated the Muescke-Schilling fully resolved DNS simulation results, with agreement between experiment and simulation. We extended this agreement to the high Schmidt number case (salt-fresh water over a splitter plate), using a fully compressible code with SGS models, and a large eddy simulation (LES), i.e., not requiring full DNS resolution. The high Schmidt number case is inaccessible to the above DNS methods.

However, not all experiments have such a high level of noise. Our analysis of the Smeeton-Youngs rocket rig (fresh-salt water) experiments suggested that they were relatively free of long wavelength noise. We simulated these, in agreement with experiment, and for the first time, with a simulation going through all experimental data points (see Fig. 1).

Our results show a clear dependence of the mixing rates on the Schmidt number. A common simulation strategy is known as Implicit Large Eddy Simulation (ILES), whereby the numerical algorithm supplies what it will for the subgrid effects, while the physical transport parameters are either zero or so small as to leave the transport effects underresolved on any feasible grid level, and thus negligible relative to numerical transport. The Schmidt number

is the ratio of viscosity to mass diffusivity. If both numerator and denominator are set to zero, the ratio is the indeterminant expression 0/0. If both are set by numerical algorithms and code artifacts, then it is a code-dependent numerical Schmidt number that is determining the answer. The result (and this was observed in practice) is two well-documented codes converging numerically to two distinct answers (see [5-7] for this and related results). Clearly this is a major challenge for V&V. The SGS models and a valid LES simulation cure this ambiguity, and allow mesh convergence, even for such sensitive and important observables as the joint probability distributions for temperature and species concentration, or for a chemical reaction rate.

The mathematical literature contains non-uniqueness theorems for the compressible Euler equations, i.e., fluid equations with fluid transport set to zero. Thus V&V for Implicit Large Eddy Simulations (ILES) has hit a mathematical no-go theorem. Obviously, a change in strategy is needed, and this is what we provide.

In comparing the Smeeton-Youngs to the Mueschke-Andrews fresh-salt water Rayleigh-Taylor mixing experiments, we found six significant differences in the experimental conditions, and all of them had a significant effect on the mixing rate (alpha). Beyond the fluid transport parameters and long-wave noise (in the Mueschke-Andrews experiment only), we found significant influence from the change in Grashov number, initial mass diffusion layer width, and experimentally induced vs. ideal short wave length perturbations.

Thus a central conclusion of our study is that there is nothing universal about Rayleigh-Taylor mixing. Many details of the experiment are important. When modeled correctly, nearly perfect agreement between simulation and experiment can be obtained. Combined with mesh convergence, this is V&V.

We also propose a scientific program for recovery in an ILES world. If front tracking to control or limit numerical mass diffusion is not part of a game plan, then it is necessary to increase the numerical viscosity so that the ratio of numerical viscosity to numerical mass diffusion agrees with the physical ratio, i.e., the numerical Schmidt number must equal the physical Schmidt number for a successful ILES simulation. The implementation of this plan, which is not without difficulties, will require a calibration step for the selection of the value for numerical viscosity. Our recommended route is to abandon this narrow interpretation of ILES, and to combine the multiphysics capabilities of ILES codes with the high quality geometrical resolution of steep concentration gradients in FronTier. To this end, a FronTier API, an application programming interface designed to support code merger is under development.

Table 1. Mesh and model errors for the joint PDFs for temperature and species concentrations and for typical gas and liquid parameter values for fluid transport. Comparison of coarse and medium to fine meshes (c to f and m to f) using sup norm for the difference of the probability distribution functions and an L1 norm for the comparison of model to simulation.

	liquid			gas		
Re	c to f	m to f	model	c to f	m to f	model
≈300	0.24	0.13	0.06	0.08	0.06	0.06
≈6000	0.07	0.06	0.07	0.09	0.05	0.05
≈600K	0.26	0.06	0.07	0.22	0.09	0.08

Going beyond the study of alpha, i.e., the outer envelope of the mixing region, we have attained mesh convergence for probability density functions (PDF) of the temperature and species concentration [1]. Due to the need for higher levels of mesh refinement for this convergence study and the plan to study the variation of physical parameters, we reduced the computational burden with a 2D study, which was of a circularly imploding Rightmyer-Meshkov instability, studied past the time of reshock. With the LES SGS regularization the convergence issues were tractable, and the mesh convergence of the PDFs was obtained. Moreover, a simple theoretical model, based on the geometry of the 50% concentration isosurface (as computed) and the laminar and turbulent (as computed) diffusion coefficients was used as an independent check on the mixing PDFs, and gave errors comparable to the mesh convergence mesh errors (see Table 1).

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